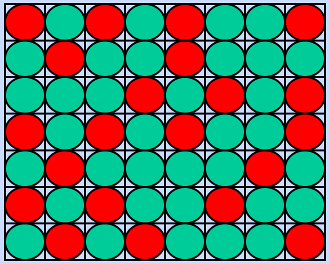
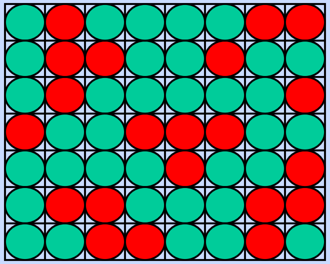
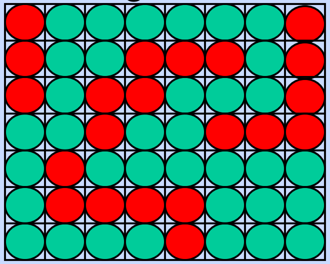
Lattice and Continuum Studies of Fluids and Fluid Mixtures

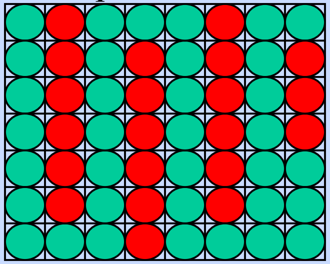
Jane E.G. Lipson   Dartmouth College   DMR-0099541





The local environment experienced by a molecule in a mixture will affect the thermodynamics, and therefore the physical behavior, of the system. Consider the the vantage point of, for example, a red segment on a lattice filled with red and green segments. In many simple (and widely-used) theories of mixtures the probability of finding a green segment in a neighboring site is just the site fraction of green, regardless of the strength of the red-red, green-green or red-green interactions. In all the examples shown, the site fraction of green is 0.62. However, only two of the four figures show sample configurations for which this represents the probability of finding a green segment next to a red. In the top right lattice (a mixture of monomers) the red segments must cluster in order to achieve the nearest-neighbor probability of 0.62 green; when distributed in an arrangement (top left) which looks more 'mixed up' the probability of having a green neighbor soars to 0.94, reflecting what may be interpreted as a relatively favorable red-green interaction. In the two bottom figures the red segments are now incorporated into hexamers. In order for the site average of 0.62 to represent the probability of finding a green next to a red the chains must be unrealistically extended, and isolated from neighboring chains. A more likely configuration, shown on the left, has a green-neighbor probability of 0.52. These examples, while clearly limited, do illustrate that in order to account for the effects of local environment both connectivity and site-site interactions should influence the probability of site occupancy. We have derived lattice and continuum theories which explore and test the role of local interactions on mixture properties and behavior. We are combining these tools with experimental data on polymer melts, solutions and blends in order to achieve a deeper understanding of structure-property relationships in complex fluids and their mixtures.





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Education:

Three undergraduates (Kallie Willets, Lisa Hall, Emily Grumbling), one graduate student (Michael Tambasco), and two postdoctoral fellows (Sergey Fridrikh and James Porter) contributed to this research. Kallie Willets is currently a graduate student at Stanford; Lisa Hall (Rose-Hulman) and Emily Grumbling (Bard) are each in their senior undergraduate year. Sergey Fridrikh is a research associate at MIT. James Porter and Michael Tambasco are currently working in the group. Two students will be joining this research: Graduate student Virginia Anderson (B.S. Willamette University), and undergraduate Adrian Accurso, who has just been awarded a Dartmouth Presidential Scholarship to start work in the group come the winter of 2004.

Outreach:

The PI engaged local grade school students in order to explore properties of solids, liquids, and gases. The effects of changing temperature (using liquid nitrogen and solid carbon dioxide) and the special properties of water (ice cubes compared to ethanol cubes) were among the interesting phenomena discussed in the context of a variety of demonstrations

Dipping a rose into liquid nitrogen and then rapidly striking the rose against the desk generated a very enthusiastic response.